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ON THE LIFETIME OF QUASI-STATIONARY STATES IN NON-RELATIVISTIC QED

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Abstract. We consider resonances in the Pauli-Fierz model of non-relativistic QED. We use and slightly modify the analysis developed by Bach, Fröhlich and Sigal [3, 4] to obtain an upper and *lower* bound on the lifetime of quasi-stationary states.

1. Introduction and Main Result

Spectral properties of models of non-relativistic QED were investigated by Bach, Fröhlich, Sigal and Soffer [1, 3, 4, 5] and by many others. Bach, Fröhlich, and Sigal [4] proved, among other things, an upper bound on the lifetime of quasi-stationary states.

We show an upper and *lower* bound on the lifetime of quasi-stationary states. We heavily rely on the analysis developed in [3, 4], but choose a different contour of integration and make use of an additional cancellation of terms. Moreover, we neither require a non-degeneracy assumption nor a spectral cutoff. However, we do not provide time dependent estimates on the remainder term and there are no photons in our quasi-stationary state. Estimates similar to ours were obtained before by different authors for other models, see e.g. [16, 17].

In order to be self-contained, we give all the necessary definitions for the model considered. For details, we refer the reader to [4]. We consider an atom in interaction with the second quantized electromagnetic field. The Hilbert space of the system is given by

$$\mathcal{H} := \mathcal{H}_{el} \otimes \mathcal{F},$$

where

$$\mathcal{H}_{el} := \mathcal{A}_N L^2[(\mathbb{R}^3 \times \mathbb{Z}_2)]^N$$

is the Hilbert space of N electrons with spin, and where

$$\mathcal{F} := \bigoplus_{N=0}^{\infty} \mathcal{S}_N L^2[(\mathbb{R}^3 \times \mathbb{Z}_2)]^N$$

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is the Fock space (with vacuum Ω) of the quantized electromagnetic field, allowing two transverse polarizations of the photon. $\mathcal{A}_N$ and $\mathcal{S}_N$ are the projections onto the subspaces of functions anti-symmetric and symmetric, respectively, under a permutation of variables. Strictly speaking, we would have to take the physical units into account in the definition of these spaces. However, we refrain from doing so in order not to complicate the notation. The operator

$$H'_{el} := -\frac{\hbar^2}{2m}\Delta_{3N} + \frac{\mathfrak{e}^2}{4\pi\epsilon_0}\left[\sum_{j=1}^{N}\frac{-\mathcal{Z}}{|x_j|} + \sum_{1\le i<j\le N}\frac{1}{|x_i - x_j|}\right]$$

describes the electrons, and the operator for the total system is

$$H'_g := \frac{1}{2m}\sum_{j=1}^{N} : [\sigma_j \cdot (-i\hbar\nabla_{x_j} - \mathfrak{e}A'_{\kappa'}(x_j))]^2 : + H'_f$$
$$+ \frac{\mathfrak{e}^2}{4\pi\epsilon_0}\left[\sum_{j=1}^{N}\frac{-\mathcal{Z}}{|x_j|} + \sum_{1\le i<j\le N}\frac{1}{|x_i - x_j|}\right],$$

where $-\mathfrak{e}\mathcal{Z}$ is the charge of the nucleus, $\mathfrak{e} < 0$ the charge of the electron, $\mathfrak{c}$ the velocity of light, $\hbar$ is Planck's constant, ϵ_0 is the permittivity of the vacuum, m the mass of the electron, σ_j is the Pauli matrix for the jth electron, and $: \cdots :$ denotes normal ordering. The kinetic energy of the photons is

$$H'_f := \hbar\mathfrak{c}\sum_{\mu=1,2}\int_{k\in\mathbb{R}^3} dk|k|a'^*_\mu(k)a'_\mu(k),$$

where the $a'^*_\mu(k)$ and $a'_\mu(k)$ are the usual creation and annihilation operators. The second quantized electromagnetic field is $A'_{\kappa'}(x) := A'_{\kappa'}(x)_+ + A'_{\kappa'}(x)_-$, where

$$A'_{\kappa'}(x)_+ := \sum_{\mu=1,2}\int dk\kappa'(|k|)\sqrt{\frac{\hbar}{2\epsilon_0\mathfrak{c}|k|(2\pi)^3}}\varepsilon'_\mu(k)e^{-ik\cdot x}a'^*_\mu(k).$$

and

$$A'_{\kappa'}(x)_- := \sum_{\mu=1,2}\int dk\kappa'(|k|)\sqrt{\frac{\hbar}{2\epsilon_0\mathfrak{c}|k|(2\pi)^3}}\varepsilon'_\mu(k)e^{ik\cdot x}a'_\mu(k).$$

Here $\varepsilon'_\mu(k)$, $\mu = 1, 2$, are the polarization vectors of the photon, depending only on the direction of k. Let us note that we use SI units here; for details about these operators, we refer the reader to [9, 10]. We set $a_0 := \alpha^{-1}(\frac{\hbar}{m\mathfrak{c}})$ (Bohr radius), $\zeta := \frac{a_0}{2}$ and $\xi^{-1} := \frac{2\alpha}{a_0}$. Moreover, $\kappa'(r) := \kappa(r\xi)$ is a cutoff function depending on the fine structure constant $\alpha = \frac{\mathfrak{e}^2}{4\pi\epsilon_0\hbar\mathfrak{c}}$. κ is a function, which is positive on $[0, \infty)$, satisfies $\kappa(r) \to 1$ as $r \to 0$, and has an analytic continuation to a cone around the positive real axis which is bounded and decays faster than any inverse polynomial, e.g., $\kappa(r) := e^{-r^4}$. Following [3], we scale the operator with the transformation $x_j \to \zeta x_j$ and $k \to \xi^{-1}k$. We denote the corresponding unitary transformation

by U. After this transformation the electron positions are measured in units of $\frac{1}{2}a_0$, photon wave vectors in units of $\frac{2\alpha}{a_0}$, and energies in units of 4Ry, where the Rydberg is Ry $:= \frac{\alpha^2 mc^2}{2}$. The creation an annihilation operators transform as

$$Ua'_\mu(k)U^{-1} = \xi^{3/2}a_\mu(\xi k), \quad Ua'^*_\mu(k)U^{-1} = \xi^{3/2}a^*_\mu(\xi k).$$

Moreover, we set

$$\varepsilon_\mu(k) := \varepsilon'_\mu(\xi^{-1}k), \quad \mu = 1,2.$$

Accordingly, we obtain

$$UH'_gU^{-1} = 2\alpha^2(mc^2)H_g,$$

with $H_g := H_0 + W_g$ and $H_0 := H_{el} \otimes \mathbf{1}_f + \mathbf{1}_{el} \otimes H_f$, where

$$H_{el} := -\Delta_{3N} + \sum_{j=1}^N \frac{-\mathcal{Z}}{|x_j|} + \sum_{1 \le i < j \le N} \frac{1}{|x_i - x_j|}.$$

Here

$$H_f := \sum_{\mu=1,2} \int_{k \in \mathbb{R}^3} dk|k|a^*_\mu(k)a_\mu(k)$$

and the interaction is given by

$$W_g := \sum_{j=1}^N \{2\alpha^{3/2}A_\kappa(\alpha x_j)\cdot(-i\nabla_{x_j}) + \alpha^3 : A^2_\kappa(\alpha x_j) : \\ + \alpha^{5/2}\sigma_j \cdot (\nabla \times A_\kappa)(\alpha x_j)\},$$

where the second quantized electromagnetic field is $A_\kappa(x) := A_\kappa(x)_+ + A_\kappa(x)_-$ with

$$A_\kappa(x)_+ := \sum_{\mu=1,2} \int \frac{dk\kappa(|k|)}{\sqrt{4\pi^2|k|}} \varepsilon_\mu(k)e^{-ik\cdot x}a^*_\mu(k).$$

and

$$A_\kappa(x)_- := \sum_{\mu=1,2} \int \frac{dk\kappa(|k|)}{\sqrt{4\pi^2|k|}} \varepsilon_\mu(k)e^{ik\cdot x}a_\mu(k).$$

As in [4], we set $g := \alpha^{3/2}$. Henceforth, we let the coupling constant $g := \alpha^{3/2} > 0$ be the perturbation parameter. We assume that the spectrum of H_{el} has the structure

$$\sigma(H_{el}) = \{E_0, E_1, \ldots\} \cup [\Sigma, \infty),$$

where $\Sigma := \inf \sigma_{ess}(H_{el})$ and $E_0 < E_1 < \ldots$ are (at least two) eigenvalues (possibly) accumulating at Σ. In the following, we will look at one (fixed) eigenvalue E_j of H_{el} with $j \ge 1$. For $0 < \epsilon < 1/3$ we set $\rho_0 := g^{2-2\epsilon}$, and $\mathcal{A}(\delta,\epsilon) := [E_j - \delta/2, E_j + \delta/2] + i[-g^{2-\epsilon}, \infty)$, where $\delta := \mathrm{dist}(E_j, \sigma(H_{el}) \setminus \{E_j\}) > 0$. We define the operators

$$H_{el}(\theta) := \mathcal{U}_{el}(\theta)H_{el}\mathcal{U}_{el}(\theta)^{-1},\ H_g(\theta) := \mathcal{U}(\theta)H_g\mathcal{U}(\theta)^{-1}, \\ W_g(\theta) := \mathcal{U}(\theta)W_g\mathcal{U}(\theta)^{-1} \tag{1}$$

for real θ, where $\mathcal{U}(\theta)$ is the unitary group associated to the generator of dilations. It is defined in such a way that the space coordinates of the electrons are dilated as $x_j \mapsto e^\theta x_j$ and the momentum coordinates of the photons as $k \mapsto e^{-\theta} k$. It can be shown [4, Corollary 1.3, Corollary 1.4] that the operators defined in equation (1) are analytic families for $|\theta| \leq \theta_0$ for some $\theta_0 > 0$. We introduce the convention $\theta := i\vartheta$ with $\vartheta > 0$. Moreover, $\mathcal{U}_{el}(\theta)$ is the above dilation acting on the electronic space only.

We define (with $r > 0$ small enough) $P_{el,i}(\theta) := -(2\pi i)^{-1} \int_{|E_i - z| = r} (H_{el}(\theta) - z)^{-1} dz$ to be the projection onto the eigenspace corresponding to the eigenvalue E_i of $H_{el}(\theta)$ and set $\overline{P}_{el,i}(\theta) := 1 - P_{el,i}(\theta)$. Furthermore, we define $P(\theta) := P_{el,j}(\theta) \otimes \chi_{H_f \leq \rho_0}$ and $\overline{P}(\theta) := 1 - P(\theta)$. We abbreviate $P_{el,i} := P_{el,i}(0)$.

Note that if we consider operators of the form PAP, where A is a closed operator and P a projection with $\operatorname{Dom} A \subset \operatorname{Ran} P$, then our notation does not distinguish between the operators PAP and $PAP|_{\operatorname{Ran} P}$. It will be clear from the context, how the symbol PAP is to be understood.

Following [4], we make crucial use of the Feshbach operator

$$
\begin{aligned}
(2) \quad \mathcal{F}_{P(\theta)}(H_g(\theta) - z) &:= P(\theta)(H_g(\theta) - z)P(\theta) \\
&\quad - P(\theta)W_g(\theta)\overline{P}(\theta)[\overline{P}(\theta)(H_g(\theta) - z)\overline{P}(\theta)]^{-1}\overline{P}(\theta)W_g(\theta)P(\theta).
\end{aligned}
$$

For the convenience of the reader, we summarize its most important properties including its existence in Appendix A. For details, we refer the reader to [3, Section IV] and [4]. It was shown in [3, 4] that the Feshbach operator can be approximated in a sense to be shown using the operators

$$
\begin{aligned}
(3) \quad \tilde{Z}_j^{od}(\alpha) := \lim_{\epsilon \downarrow 0} \sum_{\mu=1,2} \int_{k \in \mathbb{R}^3} & dk P_{el,j} w_{0,1}^{(0)}(k,\mu) \\
& \times \overline{P}_{el,j}[\overline{P}_{el,j} H_{el} - E_j + |k| - i\epsilon]^{-1} \overline{P}_{el,j} w_{1,0}^{(0)}(k,\mu) P_{el,j}
\end{aligned}
$$

and

$$
(4) \qquad \tilde{Z}_j^{d}(\alpha) := \sum_{\mu=1,2} \int_{k \in \mathbb{R}^3} \frac{dk}{|k|} P_{el,j} w_{0,1}^{(0)}(k,\mu) P_{el,j} w_{1,0}^{(0)}(k,\mu) P_{el,j}.
$$

Here the coupling functions $w_{0,1}^{(\theta)}(k,\mu)$ and $w_{1,0}^{(\theta)}(k,\mu)$ will be needed later with $\theta \neq 0$. Denoting the momentum of the jth electron by p_j, they are

$$
(5) \qquad w_{0,1}^{(\theta)}(k,\mu) := w_{1,0}^{(\bar{\theta})}(k,\mu)^* := \sum_{j=1}^{N} \{2e^{-\theta} G_{x_j}^{(\theta)}(k,\mu) \cdot p_j + \sigma_j \cdot B_{x_j}^{(\theta)}(k,\mu)\},
$$

where

$$
(6) \qquad G_x^{(\theta)}(k,\mu) := \frac{e^{-\theta} \kappa(e^{-\theta}|k|)}{\sqrt{4\pi^2 |k|}} e^{i\alpha k \cdot x} \epsilon_\mu(k)
$$

and

$$B_x^{(\theta)}(k,\mu) := \frac{\alpha e^{-2\theta}\kappa(e^{-\theta}|k|)}{i\sqrt{4\pi^2|k|}} e^{i\alpha k\cdot x}(k \times \epsilon_\mu(k)). \tag{7}$$

We set

$$\tilde{Z}(\alpha) := Z_j^d(\alpha) + Z_j^{od}(\alpha), \;\; \tilde{Z}(\alpha,\theta) := \mathcal{U}_{el}(\theta)\tilde{Z}(\alpha)\mathcal{U}_{el}(\theta)^{-1}, \\ Z(\theta) := \tilde{Z}(0,\theta), \text{ and } Z := \tilde{Z}(0,0). \tag{8}$$

We consider the Feshbach operator $\mathcal{F}_{P(\theta)}(H_g(\theta) - z)$ as an operator on $\operatorname{Ran} P(\theta)$. Similarly, we consider $\tilde{Z}(\alpha) := Z_j^d(\alpha) + Z_j^{od}(\alpha)$ and $\tilde{Z}(\alpha,\theta)$ as operators on $\operatorname{Ran} P_{el,j}$ and $\operatorname{Ran} P_{el,j}(\theta)$ respectively.

We are now able to formulate our main result. It will be proven in Section 2.

Theorem 1. *Let $0 < \epsilon < 1/3$ and g small enough. Let ϕ_1 and ϕ_2 be normalized eigenvectors of H_{el} with eigenvalue E_j and $\Phi_i := \phi_i \otimes \Omega$. Assume moreover that the imaginary part $\operatorname{Im} Z := \frac{1}{2i}(Z - Z^*)$ of Z is strictly positive on $\operatorname{Ran} P_{el,j}$. Then, in terms of a dimensionless time parameter $s \geq 0$,*

$$\langle \Phi_1, e^{-isH_g}\Phi_2\rangle = \langle \phi_1, e^{-is(E_j - g^2 Z)}\phi_2\rangle + b(g,s),$$

where $|b(g,s)| \leq C g^\epsilon$ for some $C \geq 0$.

The theorem has the following immediate Corollary:

Corollary 2. *Under the assumptions of Theorem 1, if $0 < \tau := g^2 s$ is kept fixed, if $\phi := \phi_1 = \phi_2$ are eigenvectors of Z with eigenvalue Γ, and if $\Phi := \phi \otimes \Omega$, then*

$$\lim_{g\downarrow 0} |\langle \Phi, e^{-isH_g}\Phi\rangle| = e^{-\tau \operatorname{Im}\Gamma}.$$

We close the introductory section with the following remarks:

Remark 1. The theorem can be rewritten in terms of the original operators: Let ϕ_1' and ϕ_2' be normalized eigenvectors of H_{el}' with eigenvalue $2\alpha^2 mc^2 E_j$ and $\Phi_i' := \phi_i' \otimes \Omega$. Then $\langle \Phi_1', e^{-it\hbar^{-1}H_g'}\Phi_2'\rangle = \langle \phi_1', e^{-it\frac{2\alpha^2 mc^2}{\hbar}(E_j - g^2 Z')}\phi_2'\rangle + \mathcal{O}(\alpha^{3\epsilon/2}) = \langle \phi_1, e^{-it\frac{2\alpha^2 mc^2}{\hbar}(E_j - g^2 Z)}\phi_2\rangle + \mathcal{O}(\alpha^{3\epsilon/2})$, where $\phi_i \otimes \Omega = U[\phi_i' \otimes \Omega]$.

Here

$$\begin{aligned} Z' := \frac{\hbar^2}{8\alpha^4 m^3 c^2}\Bigg[& \lim_{\epsilon\downarrow 0}\sum_{\mu=1,2}\int_{k\in\mathbb{R}^3} dk \frac{\kappa'(|k|)^2}{4\pi^2|k|} P_{el,j}'\epsilon_\mu(k)\cdot p'\overline{P}_{el,j}' \\ & \times [\overline{P}_{el,j}' H_{el}' - 2\alpha^2 mc^2 E_j + \hbar c|k| - i\epsilon]^{-1}\overline{P}_{el,j}'\epsilon_\mu(k)\cdot p' P_{el,j}' \\ & + \sum_{\mu=1,2}\int_{k\in\mathbb{R}^3}\frac{dk}{\hbar c|k|}\frac{\kappa'(|k|)^2}{4\pi^2|k|} P_{el,j}'\epsilon_\mu(k)\cdot p' P_{el,j}'\epsilon_\mu(k)\cdot p' P_{el,j}'\Bigg] \end{aligned} \tag{9}$$

$P_{el,i}'$ is the projection onto the eigenspace of H_{el}' belonging to the eigenvalue $2\alpha^2 mc^2 E_i$, $p_j' := -i\hbar\nabla_{x_j}$ and $p' := \sum_{j=1}^n p_j'$.

Remark 2. Note that the matrix $\tilde{Z}(\alpha)$ depends on the fine structure constant α, since the coupling functions defined in equations (5), (6), and (7) do. Thus, due to the exponential decay of the eigenfunctions of the electronic operator, $\tilde{Z}(\alpha)$ can be developed in a power series in $\alpha = g^{2/3}$. The zero order term corresponds to electric dipole (E1) transitions, the higher order terms to magnetic dipole transitions as well as to higher order electric and magnetic transitions. We have for some $C > 0$

$$g^2 \|\tilde{Z}(\alpha, \theta) - Z(\theta)\| \le C g^{2+2/3}. \tag{10}$$

It is easy to see that the imaginary part of Z is (see also [3, Formula (IV.19)])

$$\begin{aligned} \operatorname{Im} Z = \pi \sum_{i=0}^{j-1} \sum_{\mu=1,2} \int_{|\omega|=1} & d\omega (E_i - E_j)^2 \\ & \times \frac{4\kappa(E_j - E_i)^2}{4\pi^2 (E_j - E_i)} P_{el,j} [\epsilon_\mu(\omega) \cdot p] P_{el,i} [\epsilon_\mu(\omega) \cdot p] P_{el,j} = \\ & \qquad \frac{8}{3} \sum_{i=0}^{j-1} (E_j - E_i) \kappa(E_j - E_i)^2 P_{el,j} p P_{el,i} p P_{el,j}, \end{aligned} \tag{11}$$

In the last step we used the relationships $\sum_{\mu=1,2} (\epsilon_\mu(\omega))_m (\epsilon_\mu(\omega))_n = \delta_{m,n} - \omega_m \omega_n$ and $\int d\omega \omega_m \omega_n = \frac{4\pi \delta_{m,n}}{3}$, where $\delta_{m,n}$ is the Kronecker symbol. Moreover, $p := \sum_{j=1}^N p_j$ and the expression $P_{el,j} p P_{el,i} p P_{el,j}$ indicates a Euclidean inner product. Analogously, we set $x := \sum_{j=1}^N x_j$. Using the commutation relation

$$[x, H_{el}] = 2ip$$

we find

$$\operatorname{Im} Z = \frac{2}{3} \sum_{i=0}^{j-1} (E_j - E_i)^3 \kappa(E_j - E_i)^2 P_{el,j} x P_{el,i} x P_{el,j}. \tag{12}$$

We analyze equation (12) for the case of a hydrogen atom in Appendix B. We show there that $\operatorname{Im} Z$ is indeed strictly positive unless $j = 1$. If $j = 1$, $\operatorname{Im} Z$ has a zero eigenvalue, since the $2s$ state of hydrogen cannot decay via electric dipole transitions. However, the $2p$ states can decay via an electric dipole transition. It would be interesting to prove time decay estimates also in the latter case.

Note that the transition rate is proportional to $g^2 \alpha^2 \propto \alpha^5$, in accordance with physics textbooks (see e.g. [6, Section 59]).

Remark 3. The eigenvectors of H_{el} are analytic vectors for the generator of dilations, and therefore $\mathcal{U}_{el}(\theta) : \ker(H_{el}(0) - E_j) \to \ker(H_{el}(\theta) - E_j)$ is a (bounded and bounded invertible) mapping between finite dimensional vector spaces. (The latter is true for $|\operatorname{Im} \theta| < \pi/2$.) This implies that the matrices $Z(0)$ and $Z(\theta)$ are similar. In particular, the bounded operators $[-g^2 Z(0) \otimes \mathbf{1}_f + e^{-\theta} \mathbf{1}_{el} \otimes H_f]|_{\operatorname{Ran} P(0)}$ and $[-g^2 Z(\theta) \otimes \mathbf{1}_f + e^{-\theta} \mathbf{1}_{el} \otimes H_f]|_{\operatorname{Ran} P(\theta)}$ are similar (cf. [4, Section 3]). This fact will be used in the proof of Theorem 1 and in Section 3.

2. Proof of the Main Result

In this section we prove our main result. The technical estimates needed in the proof are collected in a series of lemmas and deferred to Section 3. For the proof we need the operator (see [3, Formula (IV.67)])

$$
\begin{aligned}
Q^{(\theta)}(z) := \sum_{\mu=1,2} \int_{k\in\mathbb{R}^3} & dk P(\theta)[w_{0,1}^{(\theta)}(k,\mu)\otimes \mathbf{1}_f] \\
& \times \left[\frac{\overline{P}(\theta)(|k|)}{H_{el}(\theta)+e^{-i\vartheta}(H_f+|k|)-z}\right][w_{1,0}^{(\theta)}(k,\mu)\otimes \mathbf{1}_f]P(\theta),
\end{aligned}
\tag{13}
$$

defined on $\operatorname{Ran} P(\theta)$ and for $z \in \mathcal{A}(\delta,\epsilon)$. Here we used the definition $\overline{P}(\theta)(|k|) := \overline{P}_{el,j}(\theta)\otimes \mathbf{1}_f + P_{el,j}(\theta)\otimes \chi_{H_f+|k|\geq\rho_0}$. Moreover, we need the the operator $Q_0^{(\theta)}(z)$ on $\operatorname{Ran} P_{el,j}(\theta)$, defined by $[Q_0^{(\theta)}(z)\phi]\otimes\Omega := Q^{(\theta)}(z)[\phi\otimes\Omega]$ for all $\phi \in \operatorname{Ran} P_{el,j}(\theta)$. It is defined by the formula

$$
\begin{aligned}
& Q_0^{(\theta)}(z) \\
&= \sum_{\mu=1,2}\int_{k\in\mathbb{R}^3} dk \chi_{|k|\geq\rho_0} P_{el,j}(\theta) w_{0,1}^{(\theta)}(k,\mu)\left[\frac{P_{el,j}(\theta)}{E_j+e^{-i\vartheta}|k|-z}\right] w_{1,0}^{(\theta)}(k,\mu)\ P_{el,j}(\theta) \\
&\quad + \sum_{\mu=1,2}\int_{k\in\mathbb{R}^3} dk P_{el,j}(\theta) w_{0,1}^{(\theta)}(k,\mu)\left[\frac{\overline{P}_{el,j}(\theta)}{H_{el}(\theta)+e^{-i\vartheta}|k|-z}\right] w_{1,0}^{(\theta)}(k,\mu)\ P_{el,j}(\theta).
\end{aligned}
\tag{14}
$$

We remark that both operators are analytic for $z \in \mathcal{A}(\delta,\epsilon)$. This follows from the fact that the resolvents in their definitions can be bounded uniformly in $z \in \mathcal{A}(\delta,\epsilon)$. (See the proof of Lemma 3 for a proof in the case of $Q_0^{(\theta)}(z)$. The proof for $Q^{(\theta)}(z)$ is similar and uses additionally the spectral theorem for H_f.)

Note that by assumption there exists a constant $c > 0$ such that $\operatorname{Im} Z \geq c$. Since Z is bounded, there are constants $a, b > 0$ such that $\operatorname{NumRan} Z$ is localized as $\operatorname{NumRan} Z \subset A(c,a,b)$, where $A(c,a,b) := ic + [-a,a] + i[0,b]$ (see Figure 2). We set $\nu := \min\{\vartheta, \arctan(c/(2a))\}$.

Finally for $w \in \mathbb{C}$ and $r > 0$ we define $D(w,r) := \{z \in \mathbb{C} | |z-w| < r\}$, and for $A \subset \mathbb{C}$ we set $D(A,r) := \{z \in \mathbb{C} | \operatorname{dist}(z,A) < r\}$. The notation $[z,w]$ denotes either the line segment between $z \in \mathbb{C}$ and $w \in \mathbb{C}$ or a linear contour from $z \in \mathbb{C}$ to $w \in \mathbb{C}$. Accordingly, $[z_1,w_1]+[z_2,w_2]$ is to be understood either as the sum of the sets $[z_1,w_1] \subset \mathbb{C}$ and $[z_2,w_2] \subset \mathbb{C}$ or as a generalized contour.

Proof of Theorem 1. First, we show that we can introduce a spectral cutoff with an error of $\mathcal{O}(g)$: We choose a function $F \in C_0^\infty((E_j-\delta/2, E_j+\delta/2))$ with $0 \leq F(x) \leq 1$ for all $x \in [E_j-\delta/2, E_j+\delta/2]$ and $F(x) = 1$ for all $x \in [E_j-\delta/4, E_j+\delta/4]$.

By the almost analytic functional calculus [14, 11]

$$
\begin{aligned}
F(H_g) &= \frac{1}{\pi}\int dxdy \frac{\tilde{F}(z)}{\bar{\partial} z}(H_g - z)^{-1} \\
&= \frac{1}{\pi}\int dxdy \frac{\tilde{F}(z)}{\bar{\partial} z}(H_0 - z)^{-1} - \frac{1}{\pi}\int dxdy \frac{\tilde{F}(z)}{\bar{\partial} z}(H_g - z)^{-1} W_g (H_0 - z)^{-1}
\end{aligned}
$$

where $\tilde{F} \in C_0^\infty(\mathbb{C})$ is an almost analytic extension of $F(x)$ with $|\frac{\tilde{F}(z)}{\partial \bar{z}}| = \mathcal{O}(|\mathrm{Im}\, z|^2)$. Since

$$
\frac{1}{\pi}\int dxdy \frac{\tilde{F}(z)}{\partial \bar{z}} \langle e^{isH_g}\Phi_1, (H_0 - z)^{-1}\Phi_2\rangle = \langle e^{isH_g}\Phi_1, \Phi_2\rangle
$$

and

$$
\begin{aligned}
&|\frac{1}{\pi}\int dxdy \langle e^{isH_g}\Phi_1, \frac{\tilde{F}(z)}{\partial \bar{z}}(H_g - z)^{-1} W_g (H_0 - z)^{-1}\Phi_2\rangle| \\
&\qquad \leq \frac{1}{\pi}\int dxdy \|\Phi_1\| |\frac{\tilde{F}(z)}{\bar{\partial} z}| \|(H_g - z)^{-1}\| |(E_j - z)^{-1}| \|W_g \Phi_2\| \leq Cg,
\end{aligned}
$$

we find that $\langle \Phi_1, e^{-isH_g}\Phi_2\rangle = \langle \Phi_1, e^{-isH_g}F(H_g)\Phi_2\rangle + \mathcal{O}(g)$.

Analogous to [15] and [4], we can write

$$
\begin{aligned}
\langle \Phi_1, e^{-isH_g}F(H_g)\Phi_2\rangle &= -\frac{1}{2\pi i}\lim_{\epsilon\downarrow 0}\int d\lambda e^{-i\lambda s}F(\lambda)[f(0,\lambda - i\epsilon) - f(0, \lambda + i\epsilon)] \\
&= -\frac{1}{2\pi i}\int d\lambda e^{-i\lambda s} F(\lambda)[f(\overline{\theta}, \lambda) - f(\theta,\lambda)],
\end{aligned}
$$

where $f(\theta,\lambda) := \langle \psi_1(\overline{\theta}), \frac{1}{H_g(\theta)-\lambda}\psi_2(\theta)\rangle$ with $\psi_i(\theta) := \phi_i(\theta)\otimes\Omega$ and $\phi_i(\theta) := \mathcal{U}_{el}(\theta)\phi_i$. We used Stone's theorem in the first step. In the second step we used the analyticity of $H_g(\theta)$ and the fact that $H_g(\theta)$ has no spectrum in the interval $[E_j - \delta/2, E_j + \delta/2]$ (see [4, Theorem 3.2] and also Corollary 8 below).

Noting that $\langle \psi_1(\overline{\theta}), \frac{1}{H_g(\theta)-\lambda}\psi_2(\theta)\rangle = \langle \psi_1(\overline{\theta}), \mathcal{F}_{P(\theta)}(H_g(\theta)-\lambda)^{-1}\psi_2(\theta)\rangle$ (see [3, Formula (IV).14] and also Lemma A.6) and using the resolvent equation, we obtain

$$
\begin{aligned}
f(\theta,\lambda) &= \langle \psi_1(\overline{\theta}), \mathcal{F}_{P(\theta)}(H_g(\theta)-\lambda)^{-1}\psi_2(\theta)\rangle \\
&= \langle \phi_1(\overline{\theta}), [E_j - \lambda - g^2 Q_0^{(\theta)}(\lambda)]^{-1}\phi_2(\theta)\rangle - \langle \psi_1(\overline{\theta}), [E_j - \lambda - g^2 Q_0^{(\theta)}(\lambda)]^{-1}\otimes \mathbf{1}_f \\
&\qquad \times [\mathcal{F}_{P(\theta)}(H_g(\theta)-\lambda) - (E_j - \lambda + e^{-\theta}\mathbf{1}_{el}\otimes H_f - g^2 Q^{(\theta)}(\lambda))P(\theta)] \\
&\qquad\qquad \times \mathcal{F}_{P(\theta)}(H_g(\theta)-\lambda)^{-1}\psi_2(\theta)\rangle =: \tilde{f}(\theta,\lambda) + B(\theta,\lambda),
\end{aligned}
$$

where $\tilde{f}(\theta,\lambda)$ is the first term in the sum. The strategy is now to move the contour for the first term in order to pick up a pole contribution (see Figure 1), and to

estimate the second term on the real axis:

$$
\begin{aligned}
&\int d\lambda e^{-i\lambda s} F(\lambda)[f(\overline{\theta},\lambda) - f(\theta,\lambda)] \\
&\quad = \int d\lambda e^{-i\lambda s} F(\lambda)[B(\overline{\theta},\lambda) - B(\theta,\lambda)] + \int\limits_{C_1+C_5} dz e^{-izs} F(z)[\tilde{f}(\overline{\theta},z) - \tilde{f}(\theta,z)] \\
&\quad + \int\limits_{C_2+C_3+C_4} dz e^{-izs}[\tilde{f}(\overline{\theta},z) - \tilde{f}(\theta,z)] - \int\limits_{C_0} dz e^{-izs}[\tilde{f}(\overline{\theta},z) - \tilde{f}(\theta,z)],
\end{aligned}
$$

where we set $C := C_1 + C_2 + C_3 + C_4 + C_5$, with $C_1 := [E_j - \delta/2, E_j - \delta/4]$, $C_2 := [E_j - \delta/4, E_j - \delta/4 - ig^{2-\epsilon}/2]$, $C_3 := [E_j - \delta/4 - ig^{2-\epsilon}/2, E_j + \delta/4 - ig^{2-\epsilon}/2]$, $C_4 := [E_j + \delta/4 - ig^{2-\epsilon}/2, E_j + \delta/4]$ and $C_5 := [E_j + \delta/4, E_j + \delta/2]$. C_0 is a suitable contour to pick up the pole contribution from $\tilde{f}(\theta,z)$. The analyticity properties required for this process will be discussed below. Note that the contour C cannot simply be moved down much further, since $Q_0^{(\theta)}(z)$ may have singularities outside of $\mathcal{A}(\delta,\epsilon)$.

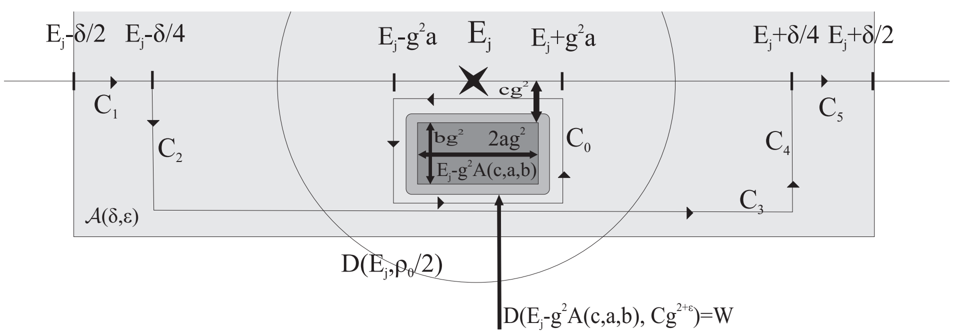

FIGURE 1. The integration contour

Estimates on the real axis: We divide the integration interval $[E_j - \delta/2, E_j + \delta/2]$ into two parts: On $[E_j - \delta/2, E_j + \delta/2] \setminus (E_j - \rho_0/2, E_j + \rho_0/2)$ we use Lemma A.7 and Lemma 7 to obtain $|B(\theta,\lambda)| \leq C \cdot \frac{g^{2+\epsilon}}{(\sin\vartheta)^2(|\lambda - E_j| - Cg^2)^2}$. Since

$$
\begin{aligned}
(\sin\vartheta)^{-2} \int\limits_{\frac{g^{2-2\epsilon}}{2}}^{\infty} \frac{d\lambda}{(\lambda - Cg^2)^2} &= (\sin\vartheta)^{-2} g^{-2} \int\limits_{\frac{g^{-2\epsilon}}{2}}^{\infty} \frac{d\lambda}{(\lambda - C)^2} \\
&= (\sin\vartheta)^{-2} g^{-2} \frac{1}{g^{-2\epsilon}/2 - C} = \mathcal{O}(\vartheta^{-2} g^{-2+2\epsilon}),
\end{aligned}
$$

we see that the error term for this region is of the order $\vartheta^{-2} g^{3\epsilon}$. On $(E_j - \rho_0/2, E_j + \rho_0/2)$ we estimate using Lemma A.7 and Lemma 6: $|B(\theta,\lambda)| \leq C\vartheta^{-2} \cdot \frac{g^{2+\epsilon}}{(E_j - \lambda)^2 + c^2 g^4}$.

Since $\int d\lambda \frac{g^{2+\epsilon}}{(E_j-\lambda)^2+c^2g^4}$ is easily seen to be of order g^ϵ, and the same estimates hold for $B(\overline{\theta},\lambda)$, the estimate on the real axis is proven.

Estimates on the contour C: We estimate the integral $\int_C |e^{-isz}||\tilde f(\overline{\theta},z) - \tilde f(\theta,z)||dz|$. Note that

$$\begin{aligned}&\tilde f(\theta,z)\\ &\quad = \frac{1}{E_j-z}\langle\phi_1(\overline{\theta}),\phi_2(\theta)\rangle + g^2\langle\phi_1(\overline{\theta}),\frac{1}{E_j-z}Q_0^{(\theta)}(z)\frac{1}{E_j-z-g^2Q_0^{(\theta)}(z)}\phi_2(\theta)\rangle.\end{aligned}$$

Thus, the zero order terms of $f(\theta,z)$ and $f(\overline{\theta},z)$ cancel each other, and it suffices to show that the higher order terms are at least of order g^ϵ. Since $Q_0^{(\theta)}(z)$ is uniformly bounded in $z\in\mathcal{A}(\delta,\epsilon)$ by Lemma 3, we estimate using Corollary 4 (see Figure 3)

$$\begin{aligned}&g^2|\langle\phi_1(\overline{\theta}),\frac{1}{E_j-(\lambda-ig^{2-\epsilon})}Q_0^{(\theta)}(\lambda-ig^{2-\epsilon})\\ &\quad\times\frac{1}{E_j-(\lambda-ig^{2-\epsilon})-g^2Q_0^{(\theta)}(\lambda-ig^{2-\epsilon})}\phi_2(\theta)\rangle| \le C\cdot\frac{g^2}{(E_j-\lambda)^2+(g^{2-\epsilon})^2}.\end{aligned}$$

Thus the integral along C_3 of the above expression is easily seen to be of order g^ϵ. The integral over the remaining contour is of order g^2, since $\mathrm{dist}(z,E_j)$ can be estimated independently of g along this part of the contour. The integral of $\tilde f(\overline{\theta},z)$ can be estimated in the same way.

Estimates on the pole term: Since $Q_0^{(\theta)}(z)$ is uniformly bounded for $z\in\mathcal{A}(\delta,\epsilon)$ by Lemma 3, the function $\tilde f(\theta,z)$ has no poles in $\mathcal{A}(\delta,\epsilon)\setminus D(E_j,\rho_0/2)$. It follows by Lemma 6 that $E_j-z-g^2Q_0^{(\theta)}(z)$ is bounded invertible if $z\in D(E_j,\rho_0/2)\setminus(E_j-g^2A(c,a,b)+D(0,C_1\cdot g^{2+\epsilon}))\subset D(E_j,\rho_0/2)\setminus[\mathrm{NumRan}(E_j-g^2Z(0))+D(0,C_1\cdot g^{2+\epsilon})]$, i.e., all poles of $\tilde f(\theta,z)$ are in the set $W:=E_j-g^2A(c,a,b)+D(0,C_1\cdot g^{2+\epsilon})$.

Moreover, by Lemma 6 we have the estimate $\|(E_j-z-g^2Q_0^{(\theta)}(z))^{-1}\|\le C\,\mathrm{dist}(z,\mathrm{NumRan}(E_j-g^2Z))^{-1}$ for some $C>0$ if $z\in D(E_j,\rho_0/2)\setminus W$. In order to estimate the pole terms, we choose a contour C_0 around W such that the length of the contour and its distance to W are of order g^2. A possible choice is $C_0=[E_j+g^2(-(a+c/2)-ic/2),E_j+g^2(+(a+c/2)-ic/2)]+[E_j+g^2((a+c/2)-ic/2),E_j+g^2(+(a+c/2)-i(b+3c/2))]+[E_j+g^2(+(a+c/2)-i(b+3c/2)),E_j+g^2(-(a+c/2)-i(b+3c/2))]+[E_j+g^2(-(a+c/2)-i(b+3c/2)),E_j+g^2(-(a+c/2)-i(c/2))]$. We now use the expansion

$$\begin{aligned}&\langle\phi_1(\overline{\theta}),(E_j-z-g^2Q_0^{(\theta)}(z))^{-1}\phi_2(\theta)\rangle=\langle\phi_1(\overline{\theta}),(E_j-z-g^2Z(\theta))^{-1}\phi_2(\theta)\rangle\\ &+g^2\langle\phi_1(\overline{\theta}),(E_j-z-g^2Q_0^{(\theta)}(z))^{-1}(Q_0^{(\theta)}(z)-Z(\theta))(E_j-z-g^2Z(\theta))^{-1}\phi_2(\theta)\rangle.\end{aligned}$$

The integral over the first term gives the claimed leading term, the second term is of order g^ϵ by Corollary A.9 and Lemma 6.

Since by the above considerations (with θ replaced by $\bar{\theta}$) the function $\tilde{f}(\overline{\theta}, z)$ has no poles in the lower half-plane, there is no pole contribution from this function (see also Remark 4). □

3. Technical Lemmas

As in [4], we need estimates on the numerical range and on the norm of the inverse of various operators. We make use of numerous results shown by Bach, Fröhlich, and Sigal [4], which are summarized in Appendix A. We use the following definitions from [4]: For $\eta > 0$ such that $E_j + \delta/2 < \Sigma - \eta$ we define $P_{disc}(\theta) := \sum_{i:E_i \leq \Sigma-\eta} P_i(\theta)$ and $\overline{P}_{disc}(\theta) := 1 - P_{disc}(\theta)$.

Since the operator valued function $Q_0^{(\theta)}$ is relevant for the location of the pole term in the time decay estimates, we need certain properties:

Lemma 3. *Let ϑ sufficiently small and $g^\epsilon/sin\vartheta \leq 1/2$. Then $Q_0^{(\theta)}(z)$ is uniformly bounded for $z \in \mathcal{A}(\delta, \epsilon)$.*

Proof. The proof follows [3, Chapter IV], using, however, the following estimates: For the first summand in equation (14), we use the estimate $|e^{-i\vartheta}|k| + E_j - z| \geq |\mathrm{Im}\,(e^{-i\vartheta}|k| + E_j - z)| \geq |\sin\vartheta|k| - g^{2-\epsilon}| \geq |\sin\vartheta| \cdot ||k| - \rho_0/2| \geq 1/2 \sin\vartheta|k|$, for $|k| \geq \rho_0$. For the second summand in (14), observe that for all E_i with $i \neq j$ we have $|E_i + e^{-\theta}|k| - z| \geq \sin\vartheta\delta/2 - g^{2-\epsilon} \geq 1/4\delta\sin\vartheta$ and that by Lemma A.1

$$\left\|(H_{el}(\theta) - (z - e^{-i\vartheta}|k|))^{-1}\overline{P}_{disc}(\theta)\right\| \leq \frac{2}{\Sigma - \eta - \mathrm{Re}\, z + \cos\vartheta|k|}.$$

□

This has the following immediate corollary:

Corollary 4. *There exists a constant $C > 0$ such that for all $z \in \mathcal{A}(\delta, \epsilon)$*

$$\mathrm{NumRan}(E_j - g^2 Q_0^{(\theta)}(z)) \subset D(E_j, C \cdot g^2).$$

We use the following lemma to estimate the inverse of the Feshbach operator:

Lemma 5. *Suppose A is a bounded operator on a Banach space and let A' be similar to A, i.e., there exists a bounded, bounded invertible operator G such that $A' = GAG^{-1}$. Moreover, let B be a another bounded operator. Then for any $q > 1$ and for all $z \notin D(\mathrm{NumRan}(A), q \cdot \|B\|\|G\| \cdot \|G^{-1}\|)$ the following estimate holds:*

$$\left\|(A' + B - z)^{-1}\right\| \leq \|G\| \cdot \|G^{-1}\| \frac{q}{q-1} \cdot \mathrm{dist}(z, \mathrm{NumRan}(A))^{-1}.$$

In particular, $\sigma(A' + B) \subset D(\mathrm{NumRan}(A), q \cdot \|B\|\|G\| \cdot \|G^{-1}\|)$.

Proof. First, observe that for all $z \notin \mathrm{NumRan}(A)$ by similarity

$$\|(A' - z)^{-1}\| \leq \|G\| \cdot \|G^{-1}\| \cdot \|(A - z)^{-1}\| \leq \|G\| \cdot \|G^{-1}\| \cdot \mathrm{dist}(z, \mathrm{NumRan}(A))^{-1}.$$

By a series expansion we obtain for $z \notin D(\mathrm{NumRan}(A), q \cdot \|B\| \cdot \|G\| \cdot \|G^{-1}\|)$

$$(A' + B - z)^{-1} = (A' - z)^{-1} \sum_{n=0}^{\infty} [-B(A' - z)^{-1}]^n.$$

Taking the norm of both sides implies the claim. □

Following [4], we control the Feshbach operator $\mathcal{F}_{P(\theta)}(H_g(\theta) - z)$ for $z \in D(E_j, \rho_0/2)$ as follows (see Figure 2):

Lemma 6. *Let $0 < \vartheta < \theta_0$ and $0 < g \ll \vartheta$ small enough. Then the following statements hold:*

a) *There are constants $C_1, C_2 > 0$ such that $\mathcal{F}_{P(\theta)}(H_g(\theta) - z)$ is bounded invertible for all $z \in D(E_j, \rho_0/2) \setminus D(\mathrm{NumRan}(E_j - g^2 Z(0) \otimes \mathbf{1}_f + e^{-\theta} \mathbf{1}_{el} \otimes H_f)|_{\mathrm{Ran}\, P(0)}, C_1 \cdot g^{2+\epsilon})$, and for $\lambda \in [E_j - \rho_0/2, E_j + \rho_0/2]$ the estimate*

$$\left\| \mathcal{F}_{P(\theta)}(H_g(\theta) - \lambda)^{-1} \right\| \leq \frac{C_2}{\sin \nu \sqrt{(E_j - \lambda)^2 + c g^4}}$$

holds. The same holds for $(E_j - z - g^2 Q^{(\theta)}(z) \otimes \mathbf{1}_f + e^{-\theta} \mathbf{1}_{el} \otimes H_f)|_{\mathrm{Ran}\, P(\theta)}$.

b) *There is a constant $C > 0$ such that for all $z \in \mathbb{C} \setminus \mathrm{NumRan}(E_j - g^2 Z(0))|_{\mathrm{Ran}\, P_{el,j}(0)}$ the operator $(E_j - z - g^2 Z(\theta))|_{\mathrm{Ran}\, P_{el,j}(\theta)}$ is bounded invertible and fulfills the estimate*

$$\| [(E_j - z - g^2 Z(\theta))|_{\mathrm{Ran}\, P_{el,j}(\theta)}]^{-1} \| \leq \frac{C}{\mathrm{dist}(z, \mathrm{NumRan}(E_j - g^2 Z(0))|_{\mathrm{Ran}\, P_{el,j}(0)})}. \tag{15}$$

There are constants $C_1, C_2 > 0$ such that for all $z \in D(E_j, \rho_0/2) \setminus D(\mathrm{NumRan}(E_j - g^2 Z(0))|_{\mathrm{Ran}\, P_{el,j}(0)}, C_1 \cdot g^{2+\epsilon})$ the operator $(E_j - z - g^2 Q_0^{(\theta)}(z))|_{\mathrm{Ran}\, P_{el,j}(\theta)}$ is bounded invertible and fulfills

$$\| [(E_j - z - g^2 Q_0^{(\theta)}(z))|_{\mathrm{Ran}\, P_{el,j}(\theta)}]^{-1} \| \leq \frac{C_2}{\mathrm{dist}(z, \mathrm{NumRan}(E_j - g^2 Z(0))|_{\mathrm{Ran}\, P_{el,j}(0)})}. \tag{16}$$

Proof. By similarity (cf. Remark 3) we obtain immediately for some $C_3 > 0$ that

$$\begin{aligned} &\| [(E_j - z - g^2 Z(\theta) \otimes \mathbf{1}_f + e^{-\theta} \mathbf{1}_{el} \otimes H_f)|_{\mathrm{Ran}\, P(\theta)}]^{-1} \| \\ &\qquad \leq C_1 \cdot \mathrm{dist}(z, \mathrm{NumRan}(E_j - g^2 Z(0) \otimes \mathbf{1}_f + e^{-\theta} \mathbf{1}_{el} \otimes H_f)|_{\mathrm{Ran}\, P(0)})^{-1}. \end{aligned}$$

By Lemma A.7, Corollary A.9, and Lemma 5 there are constants $C_1, C_2 > 0$ such that

$$\begin{aligned} &\| \mathcal{F}_{P(\theta)}(H_g(\theta) - z)^{-1} \| \\ &\qquad \leq C_2 \, \mathrm{dist}(z, \mathrm{NumRan}(E_j - g^2 Z(0) \otimes \mathbf{1}_f + e^{-\theta} \mathbf{1}_{el} \otimes H_f)|_{\mathrm{Ran}\, P(0)})^{-1} \end{aligned} \tag{17}$$

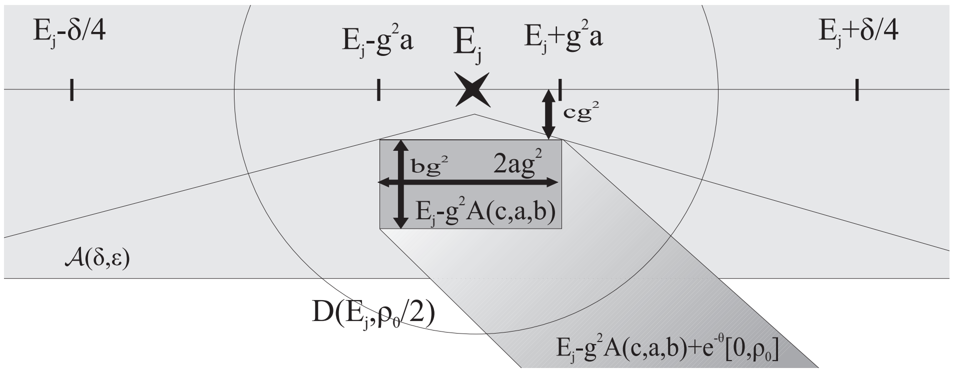

FIGURE 2. The numerical ranges of the operators $E_j - g^2 Z(0)$ and $\mathrm{NumRan}(E_j - g^2 Z(0) \otimes \mathbf{1}_f + e^{-\theta}\mathbf{1}_{el} \otimes H_f)|_{\mathrm{Ran}\, P(0)}$

follows for $z \notin D(\mathrm{NumRan}(E_j - g^2 Z(0) \otimes \mathbf{1}_f + e^{-\theta}\mathbf{1}_{el} \otimes H_f)|_{\mathrm{Ran}\, P(0)}), C_1 \cdot g^{2+\epsilon})$. It follows that $\mathrm{NumRan}[(-g^2 Z(0) \otimes \mathbf{1}_f + e^{-\theta}\mathbf{1}_{el} \otimes H_f)|_{\mathrm{Ran}\, P(0)}] \subset -g^2 A(c,a,b) + e^{-\theta}[0,\rho_0]$ (see Figure 2). By geometrical considerations, we see that this set is contained in the conical region $-i\frac{c}{2}g^2 - i\{re^{i\phi}| -(\nu - \frac{\pi}{2}) \leq \phi \leq \nu - \frac{\pi}{2}, r \in [0,\infty)\}$. This, in turn, implies the claim. The claims in b) follow by the same reasoning. □

We do not see that the estimate of Lemma 6 a) is true for $\lambda \in [E_j - \delta/2, E_j + \delta/2] \setminus (E_j - \rho_0/2, E_j + \rho_0/2)$ as used in [4, Proof of Theorem 3.5] (see also the remark after Lemma A.8). Thus we bound $\mathcal{F}_{P(\theta)}(H_g(\theta) - \lambda)^{-1}$ differently in that region in the next lemma.

Lemma 7. *Let $0 < \vartheta < \theta_0$ and $0 < g \ll \vartheta$ small enough. Then $\mathcal{F}_{P(\theta)}(H_g(\theta) - z)$ is bounded invertible for all $z \in \mathcal{A}(\delta,\epsilon) \setminus D(E_j, \rho_0/2)$ and there is a constant $C > 0$ such that for g small enough and $z \in \mathcal{A}(\delta,\epsilon) \setminus D(E_j, \rho_0/2)$ the numerical range of $\mathcal{F}_{P(\theta)}(H_g(\theta) - z)$ is localized as*

$$\mathrm{NumRan}(\mathcal{F}_{P(\theta)}(H_g(\theta) - z) + z) \subset D(E_j + e^{-\theta}[0,\rho_0], Cg^2).$$

In particular, for $\lambda \in [E_j - \delta/2, E_j + \delta/2] \setminus (E_j - \rho_0/2, E_j + \rho_0/2)$ the estimate

$$\|\mathcal{F}_{P(\theta)}(H_g(\theta) - \lambda)^{-1}\| \leq \frac{1}{\sin\vartheta(|\lambda - E_j| - Cg^2)}$$

holds. Analogous statements hold with $\mathcal{F}_{P(\theta)}(H_g(\theta) - z)$ replaced by $E_j - z - g^2 Q_0^{(\theta)}(z)$.

Proof of Lemma 7. We have by Lemma A.7 that $\|P(\theta)W_g(\theta)P(\theta)\| = \mathcal{O}(g^{2+\epsilon})$. Therefore, it suffices to show that

$$\|P(\theta)W_g(\theta)\overline{P}(\theta)[\overline{P}(\theta)(H_g(\theta) - z)\overline{P}(\theta)]^{-1}\overline{P}(\theta)W_g(\theta)P(\theta)\| = \mathcal{O}(g^2).$$

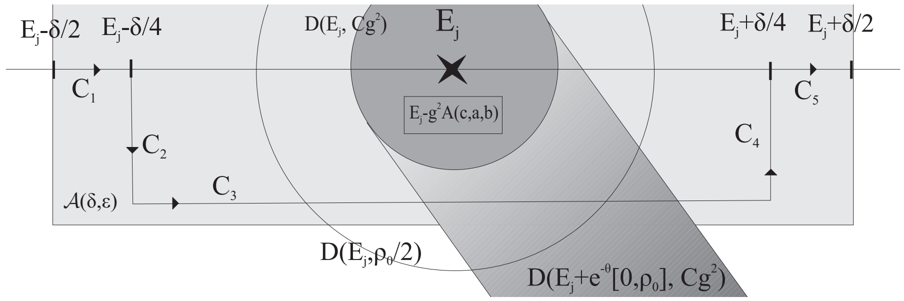

FIGURE 3. Global localization of the numerical range of $E_j + g^2 Q_0^{(\theta)}(z)$ and of the Feshbach operator $\mathcal{F}_{P(\theta)}(H_g(\theta) - z) + z$.

Following [4, Proof of Lemma 3.14], we use a Neumann expansion:

$$
\begin{aligned}
(18)\quad & \overline{P}(\theta)[\overline{P}(\theta)(H_g(\theta)-z)\overline{P}(\theta)]^{-1}\overline{P}(\theta) \\
&= \sum_{n=0}^{\infty} \overline{P}(\theta)[\overline{P}(\theta)(H_0(\theta)-z)\overline{P}(\theta)]^{-1}\overline{P}(\theta) \\
&\quad \times \left[-\overline{P}(\theta)W_g(\theta)\overline{P}(\theta)\left[\overline{P}(\theta)(H_0(\theta)-z)\overline{P}(\theta)\right]^{-1}\overline{P}(\theta)\right]^n
\end{aligned}
$$

This expansion is valid if $z \in \mathcal{A}(\delta,\epsilon)$ with $\operatorname{Im} z \geq C$ for some $C > 0$ (independent of g.) We define $B_\theta(\rho) := H_{el}(\theta) \otimes \mathbf{1}_f - E_j + e^{-\theta}(\mathbf{1}_{el} \otimes H_f + \rho)$ as in [4]. The right handside of equation (18) is equal to

$$
\begin{aligned}
(19)\quad & \sum_{n=0}^{\infty} |B_\theta(\rho_0)|^{-1/2}|B_\theta(\rho_0)|^{1/2}\overline{P}(\theta)\left[\overline{P}(\theta)(H_0(\theta)-z)\overline{P}(\theta)\right]^{-1}\overline{P}(\theta)|B_{\bar\theta}(\rho_0)|^{1/2} \\
&\quad \times \Big[-|B_{\bar\theta}(\rho_0)|^{-1/2}W_g(\theta)|B_\theta(\rho_0)|^{-1/2}|B_\theta(\rho_0)|^{1/2}\overline{P}(\theta) \\
&\quad \times \left[\overline{P}(\theta)(H_0(\theta)-z)\overline{P}(\theta)\right]^{-1}\overline{P}(\theta)|B_{\bar\theta}(\rho_0)|^{1/2}\Big]^n |B_{\bar\theta}(\rho_0)|^{-1/2} =: R(z).
\end{aligned}
$$

for all $z \in \mathcal{A}(\delta,\epsilon)$ with $\operatorname{Im} z \geq C$. By Lemma A.4 and Corollary A.3 the series in equation (19) converges uniformly for $z \in \mathcal{A}(\delta,\epsilon)$ and is thus a holomorphic function of $z \in \mathcal{A}(\delta,\epsilon)$. Thus

$$\overline{P}(\theta)[\overline{P}(\theta)(H_g(\theta)-z)\overline{P}(\theta)]^{-1}\overline{P}(\theta) = R(z)$$

for all $z \in \mathcal{A}(\delta,\epsilon)$ by holomorphic continuation and for all $z \in \mathcal{A}(\delta,\epsilon)$

$$
\begin{aligned}
(20)\quad & P(\theta)W_g(\theta)\overline{P}(\theta)\left[\overline{P}(\theta)(H_g(\theta)-z)\overline{P}(\theta)\right]^{-1}\overline{P}(\theta)W_g(\theta)P(\theta) \\
&= P(\theta)|B_{\bar\theta}(\rho_0)|^{1/2}|B_{\bar\theta}(\rho_0)|^{-1/2}W_g(\theta)R(z)W_g(\theta)|B_\theta(\rho_0)|^{-1/2}|B_\theta(\rho_0)|^{1/2}P(\theta).
\end{aligned}
$$

Note that $\||B_\theta(\rho_0)|P(\theta)\| = \|B_\theta(\rho_0)P(\theta)\|$ and $\|P(\theta)|B_{\bar\theta}(\rho_0)|\| = \|P(\theta)B_\theta(\rho_0)\|$. Thus, using $\|P(\theta)|B_{\bar\theta}(\rho_0)|^{1/2}\| \leq \|P(\theta)|B_{\bar\theta}(\rho_0)|\| \cdot \||B_{\bar\theta}(\rho_0)|^{-1/2}\| = \mathcal{O}(\rho_0^{1/2})$, and counting the powers of ρ_0 in (20), the first claim follows. The estimate on the

inverse follows by geometrical considerations. The claim on $E_j - z - g^2 Q_0^{(\theta)}(z)$ follows from Lemma 3. ☐

Note that due to the appearance of the interaction $W_g(\theta)$ on both sides of the resolvent $[\overline{P}(\theta)(H_g(\theta)-z)\overline{P}(\theta)]^{-1}$ and due to the projections $P(\theta)$, the divergence of the resolvent for $\rho_0 \to 0$ is completely eliminated (see also the remark after Lemma A.6).

We use the following corollary instead of [4, Theorem 3.2].

Corollary 8. *Let $0 < \vartheta < \theta_0$ and $0 < g \ll \vartheta$ small enough. Then*

$$\mathcal{A}(\delta, \epsilon) \setminus (E_j - D(g^2 A(c,a,b), C \cdot g^{2+\epsilon}) + e^{-\theta}[0, \rho_0]) \subset \rho(H_g(\theta))$$

for some $C > 0$. In particular, the interval $[E_j - \delta/2, E_j + \delta/2]$ is contained in the resolvent set $\rho(H_g(\theta))$.

Proof. By Lemma 7, $\mathcal{F}_{P(\theta)}(H_g(\theta) - z)$ is bounded invertible for all $z \in \mathcal{A}(\delta, \epsilon) \setminus D(E_j, \rho_0/2)$. By Lemma 6, it is bounded invertible for all $z \in D(E_j, \rho_0/2) \setminus D(\mathrm{NumRan}(E_j - g^2 Z(0) \otimes \mathbf{1}_f + e^{-\theta}\mathbf{1}_{el} \otimes H_f)|_{\mathrm{Ran}\, P(0)}, C_1 \cdot g^{2+\epsilon})$. Lemma A.6 implies the claim. ☐

Appendix A. Estimates Taken from Bach, Fröhlich, and Sigal [4]

In the appendix, we quote some important technical lemmas from [4], which we frequently use. We do not give their proofs, since they are very lengthy. However, for the orientation of the reader, we describe the essential points of the proofs in words.

A.1. **Existence of the Feshbach Operator.**

First we need certain relative bounds on the interaction and bounds on the resolvent.

Lemma A.1 ([4], Lemma 3.8)**.** *Let $z \in \mathbb{C}$ with $\mathrm{Re}\, z < \Sigma - \eta$. Then, for $|\theta|(1 + (\Sigma - \eta - \mathrm{Re}\, z)^{-1})$ sufficiently small, $H_{el}(\theta) - z$ is invertible on $\mathrm{Ran}\, \bar{P}_{disc}(\theta)$ and*

$$\left\|(\bar{P}_{disc}(\theta) H_{el}(\theta) \bar{P}_{disc}(\theta) - z)^{-1} \bar{P}_{disc}(\theta)\right\| \leq 2(\Sigma - \eta - \mathrm{Re}\, z)^{-1}$$

This lemma is proved by using that the estimate holds for $\theta = 0$ with constant one (instead of two) and using that $H_{el}(0) - H_{el}(\theta)$ is relatively $H_{el}(0)$ bounded. We remind the reader that as in [4] we define $B_\theta(\rho) := H_{el}(\theta) \otimes \mathbf{1}_f - E_j + e^{-\theta}(\mathbf{1}_{el} \otimes H_f + \rho)$. Note that $\mathcal{A}(\delta, \epsilon) \subset \rho(\overline{P}(\theta) H_0(\theta))$.

Lemma A.2 ([4], Lemma 3.11)**.** *There exists a constant $C > 0$ such that for $0 < \vartheta < \theta_0$, for all g with $0 \leq g\rho_0^{-1/2} \leq 1/3$ and $0 < \rho_0 \leq (\delta/3)\sin\vartheta$, and for all $z \in \mathcal{A}(\delta, \epsilon)$*

$$\|B_\theta(\rho_0) \frac{\overline{P}(\theta)}{H_0(\theta) - z}\| \leq \frac{C}{\vartheta}. \tag{21}$$

The proof of Lemma A.2 is based on Lemma A.1, the fact that $H_{el}(\theta)$ restricted to $P_{disc}(\theta)$ is similar to a self-adjoint operator, and various other estimates on the resolvent of $H_{el}(\theta)$ as well as the application of the spectral theorem for H_f.
The following Corollary was used in [2]:

Corollary A.3. *There exists a constant $C > 0$ such that for $0 < \vartheta < \theta_0$, all g with $0 \leq g\rho_0^{-1/2} \leq 1/3$ and $0 < \rho_0 \leq (\delta/3)\sin\vartheta$, and for all $z \in \mathcal{A}(\delta, \epsilon)$*

$$\| |B_\theta(\rho_0)|^{1/2} \frac{\overline{P}(\theta)}{H_0(\theta) - z} |B_{\bar{\theta}}(\rho_0)|^{1/2} \| \leq \frac{C}{\vartheta}.$$

Proof. By taking adjoints in equation (21), we find that $\| \frac{\overline{P}(\theta)}{H_0(\theta)-z} |B_{\bar{\theta}}(\rho_0)| \| \leq \frac{C}{\vartheta}$. The claim follows by complex interpolation. □

Lemma A.4 ([4], Lemma 3.13)**.** *There is a constant $C > 0$ such that for $0 < \vartheta < \theta_0$ sufficiently small, $\theta_1, \theta_2 \in \{\pm i\vartheta\}$ and for all $\rho > 0$*

$$\| |B_{\theta_1}(\rho)|^{-1/2} W_g(\theta) |B_{\theta_2}(\rho)|^{-1/2} \| \leq g \frac{C}{\vartheta}(1 + \rho^{-1/2}). \tag{22}$$

The proof of Lemma A.4 uses that $\|A_\kappa(x)_- \psi\| \leq C \|H_f^{1/2}\psi\|$ and $\|A_\kappa(x)_+\psi\| \leq C\|(H_f + 1)^{1/2}\psi\|$ for some $0 < C$ and all ψ in the domain of $H_f^{1/2}$, that $H_{el}(0) - H_{el}(\theta)$ is relatively $H_{el}(0)$ bounded, and some other estimates. The term proportional to $\rho^{-1/2}$ is due to the $+1$ in the bound for the creation operator $A_\kappa(x)_+$ and to the appearance of a similar constant in the estimate for the relative boundedness of $H_{el}(0) - H_{el}(\theta)$. Note that the symmetric form of the estimate (22) is essential. Estimates on $W_g(\theta)|B_{\theta_2}(\rho)|^{-1}$lead to worse behavior as $\rho \to 0$.

Lemma A.5 ([4], Lemma 3.14)**.** *There is a $C > 0$ such that for $\vartheta \in (0, \theta_0)$, $\rho_0 < (\delta/3)\sin\vartheta$, $0 < g\rho_0^{-1/2} \ll \vartheta^2$, and for all $z \in \mathcal{A}(\delta, \epsilon)$ the operator $\overline{P}(\theta)H_g\overline{P}(\theta) - z$ is invertible on $\operatorname{Ran}\overline{P}(\theta)$ and fulfills*

$$\| [\overline{P}(\theta) H_g(\theta) \overline{P}(\theta) - z]^{-1} \overline{P}(\theta) \| \leq \frac{C}{\vartheta\rho_0}.$$

The proof of Lemma A.5 uses Corollary A.3, Lemma A.4 and a Neumann series expansion.

Lemma A.6 ([4], Lemma 3.15)**.** *Assume that $\vartheta \in (0, \theta_0)$. Let $\rho_0 < (\delta/3)\sin\vartheta$ and $0 < g\rho_0^{-1/2} \ll \vartheta^2$. Then for all $z \in \mathcal{A}(\delta, \epsilon)$ the Feshbach operator $\mathcal{F}_{P(\theta)}(H_g(\theta) - z)$ defined in equation (2) exists. If $z \in \mathcal{A}(\delta, \epsilon)$, then $H_g(\theta) - z$ is bounded invertible if and only if the Feshbach operator $\mathcal{F}_{P(\theta)}(H_g(\theta) - z)$ is bounded invertible, and the equation*

$$\begin{aligned} (H_g(\theta) - z)^{-1} = {} & [P(\theta) - \overline{P}(\theta)(\overline{P}(\theta)H_g(\theta)\overline{P}(\theta) - z)^{-1}\overline{P}(\theta)W_g(\theta)P(\theta)] \\ & \times \mathcal{F}_{P(\theta)}(H_g(\theta) - z)^{-1}[P(\theta) - P(\theta)W_g(\theta)\overline{P}(\theta)(\overline{P}(\theta)H_g(\theta)\overline{P}(\theta) - z)^{-1}\overline{P}(\theta)] \\ & + \overline{P}(\theta)[\overline{P}(\theta)H_g(\theta)\overline{P}(\theta) - z]^{-1}\overline{P}(\theta) \end{aligned} \tag{23}$$

holds, where the left side exists if and only if the right side exists. Moreover, there is a constant $C > 0$, independent of g and θ, such that for all $z \in \mathcal{A}(\delta, \epsilon)$

$$\|(\overline{P}(\theta)H_g(\theta)\overline{P}(\theta) - z)^{-1}\overline{P}(\theta)W_g(\theta)P(\theta)\| \leq \frac{Cg}{\vartheta \rho_0^{1/2}} \tag{24}$$

and

$$\|P(\theta)W_g(\theta)\overline{P}(\theta)(\overline{P}(\theta)H_g(\theta)\overline{P}(\theta) - z)^{-1}\| \leq \frac{Cg}{\vartheta \rho_0^{1/2}}. \tag{25}$$

Equations (24) and (25) are proved similarly as Lemma A.5. Together with Lemma A.5 they imply the existence of the Feshbach operator and the validity of Equation (23) (see [3, Theorem IV.1]). Note that the operator $W_g(\theta)$ in Formulas (24) and (25) reduces the divergence as $\rho_0 \to 0$ in comparison to Lemma A.5.

A.2. **Approximations of the Feshbach Operator.** The following lemma gives an approximation of the Feshbach operator globally for all $z \in \mathcal{A}(\delta, \epsilon)$ (see [4], Lemma 3.16, estimates on Rem_0 through Rem_3):

Lemma A.7. *Let $0 < \epsilon < 1/3$ and $0 < \vartheta < \theta_0$. Then there is a constant $C \geq 0$ such that for all $g > 0$ sufficiently small with $\rho_0 < (\delta/3)\ sin\vartheta$, and for all $z \in \mathcal{A}(\delta, \epsilon)$*

$$\|[\mathcal{F}_{P(\theta)}(H_g(\theta) - z) - (E_j - z + e^{-\theta}\mathbf{1}_{el} \otimes H_f - g^2 Q^{(\theta)}(z))]P(\theta)\| \leq Cg^{2+\epsilon}.$$

Moreover $\|P(\theta)W_g(\theta)P(\theta)\| = \mathcal{O}(g^{2+\epsilon})$.

The lengthy and technical proof of Lemma A.7 is based on a Neumann series expansion, estimates similar to Lemma A.4, and the pull-through formula.

For z sufficiently close to E_j, $Q^{(\theta)}(z)$ can be approximated by $\tilde{Z}(\alpha, \theta)$ (see [4, Lemma 3.16, Estimates on Rem_4 and Rem_5]).

Lemma A.8. *Let $0 < \epsilon < 1/3$ and $0 < \vartheta < \theta_0$. Then there is a constant $C \geq 0$ such that for all $g > 0$ sufficiently small with $\rho_0 < (\delta/3)\ sin\vartheta$, and for all $z \in D(E_j, \rho_0/2)$*

$$g^2\|Q^{(\theta)}(z) - \tilde{Z}(\alpha, \theta)\| \leq Cg^{2+\epsilon}.$$

The proof requires some additional estimates to eliminate the z-dependence of $Q^{(\theta)}(z)$. However, we not see that Lemma A.8 holds for all $z \in \mathcal{A}(\delta, \epsilon)$, which seems to be used in [4].

Lemma A.8 and Equation (10) imply

Corollary A.9. *Under the assumptions of Lemma A.8*

$$g^2\|Q^{(\theta)}(z) - Z(\theta)\| \leq Cg^{2+\epsilon}.$$

Remark 4. Note that in order to approximate the Feshbach operator $\mathcal{F}_{P(\bar{\theta})}(H_g(\bar{\theta}) - z)$ for $\theta = i\vartheta$ with $\vartheta > 0$, the $-i\epsilon$ in definition (3) has to be replaced by $+i\epsilon$. In particular, when considering the spectral analysis of this operator, the localization of the numerical range and of the spectrum have to be reflected about the real axis.

Appendix B. The Hydrogen Atom

In this section we discuss the applicability of the presented method to the hydrogen atom. In particular, we show that $\operatorname{Im} Z$ is strictly positive unless $j = 1$. For compatibility with physics literature, we number the eigenvalues of the hydrogen atom according to the principal quantum number $n = i + 1$. We denote the corresponding eigenvalues by $\mathfrak{E}_n$, i.e., $\mathfrak{E}_n = E_i$ for all $i \geq 0$. We will ignore the (trivial) spin dependence of $Z = \tilde{Z}(0,0)$ in this appendix.

B.1. **The Hydrogen Eigenfunctions.** We define the associated Laguerre polynomials (see [6, Formula (3.5)]) for $\lambda, \mu \in \mathbb{N}_0$ with $0 \leq \mu \leq \lambda$ by

$$L_\lambda^\mu(r) := \left(\frac{d}{dr}\right)^\mu \left(e^r \left(\frac{d}{dr}\right)^\lambda \left(e^{-r} r^\lambda\right)\right)$$

and set (see [6, Formula (3.16)])

$$R_{n,l}(r) := -\frac{1}{\sqrt{8}} \frac{(n-l-1)!^{1/2}}{(n+l)!^{3/2}(2n)^{1/2}} (2/n)^{3/2} e^{-r/(2n)} \left(\frac{r}{n}\right)^l L_{n+l}^{2l+1}(r/n). \tag{26}$$

Note that the Hamiltonian in [6] has an additional factor of 1/2 in front of the Laplacian, so that the radial functions and certain other quantities have to be adapted accordingly. We would like to warn the reader that there are different conventions for the indices of the associated Laguerre functions.

For $n \in \mathbb{N}$ and $l, m \in \mathbb{Z}$ with $0 \leq l \leq n-1$ and $-l \leq m \leq l$ the normalized eigenfunctions to the eigenvalue $\mathfrak{E}_n$ are

$$u_{n,l,m}(r,\theta,\phi) := R_{n,l}(r) Y_{l,m}(\theta,\phi), \tag{27}$$

where the $Y_{l,m}$ are spherical harmonics (see [6, Section 1]) and we introduced polar coordinates by

$$\begin{aligned} x &= r \sin\theta \cos\phi \\ y &= r \sin\theta \sin\phi \\ z &= r \cos\theta \end{aligned}$$

with $0 \leq \theta \leq \pi$ and $0 \leq \phi \leq 2\pi$. Note that in this appendix x, y, and z denote the cartesian coordinates of the electron, contrary to the main part of the paper, where x and z have different meanings. Moreover, note that the eigenvalues $\mathfrak{E}_n$ are n^2-fold degenerate.

B.2. **Selection Rules for Dipole Transitions.** In this subsection, we give some important results from [6]. We define

$$R_{n,l}^{n',l'} := \int_0^\infty dr r^3 R_{n',l'}(r) R_{n,l}(r). \tag{28}$$

These integrals have been evaluated by Gordon [13] (see also [6, Section 63]). Below, we need (see [6, Formula (63.4)])

$$|R_{2,1}^{n,0}| = 2 \cdot \sqrt{\frac{2^{15} n^9 (n-2)^{2n-6}}{3(n+2)^{2n+6}}}. \tag{29}$$

For the dipole moments $(u_{n',l',m'}, z u_{n,l,m})$ one finds (see [6, Formula (60.11)]) for all $n, n' \in \mathbb{N}_0$ that

$$(u_{n',l',m'}, z u_{n,l,m}) = 0 \quad \text{unless } l' = l \pm 1 \text{ and } m' = m. \tag{30}$$

Moreover, we will need the relation

$$(u_{n',0,0}, z u_{2,1,0}) = \sqrt{\frac{1}{3}} R_{2,1}^{n',0}. \tag{31}$$

The selection rules given in [6, Formula (60.11)] imply immediately

$$(u_{n',l',m'}, x u_{n,l,m}) = (u_{n',l',m'}, y u_{n,l,m}) = 0 \tag{32}$$

unless $l' = l \pm 1$ and $m' = m \pm 1$

B.3. **The Imaginary Part of Z.** In this subsection, we show that the method presented in this paper applies to the hydrogen atom, except for the case $n = 2$.

Theorem B.1. *Fix $n \in \mathbb{N}$ and consider*

$$\begin{aligned} \operatorname{Im} Z = \frac{1}{6\pi} \sum_{i=0}^{j-1} (E_j - E_i)^3 \kappa (E_j - E_i)^2 & \\ \times [P_{el,j} x P_{el,i} x P_{el,j} + P_{el,j} y P_{el,i} y P_{el,j} + P_{el,j} z P_{el,i} z P_{el,j}] & \end{aligned}$$

for $j = n-1$ as in equation (12). Then for all $l, m, l', m' \in \mathbb{N}_0$ with $0 \le l \le n-1$, $-l \le m \le l$, $0 \le l' \le n-1$, and $-l' \le m' \le l'$

$$(u_{n,l',m'}, \operatorname{Im} Z u_{n,l,m}) = 0$$

unless $l = l'$ and $m = m'$, and for all $l, m \in \mathbb{N}_0$ with $0 \le l \le n-1$, $-l \le m \le l$

$$(u_{n,l,m}, \operatorname{Im} Z u_{n,l,m}) > 0$$

unless $n = 2$. In particular, $\operatorname{Im} Z$ *is positive, unless $n = 2$.*

Proof. Off-diagonal matrix elements: Since $\operatorname{Im} Z$ is invariant under rotations, it is diagonal in the basis $\{u_{n,l,m} | \, 0 \le l \le n-1, \, -l \le m \le l\}$. This can also be verified using the explicit formulas for the dipole matrix elements in [6, Section 63] . Note that the matrices $P_{el,j} x P_{el,i} x P_{el,j}$, $P_{el,j} y P_{el,i} y P_{el,j}$, and $P_{el,j} z P_{el,i} z P_{el,j}$ are not diagonal separately. We would like to mention that also the real part is diagonal in the basis $\{u_{n,l,m} | \, 0 \le l \le n-1, \, -l \le m \le l\}$.
Diagonal matrix elements: Let us first remark that the matrix element

$$(u_{2,0,0}, [P_{el,1} x P_{el,0} x P_{el,1} + P_{el,1} y P_{el,0} y P_{el,1} + P_{el,1} z P_{el,0} z P_{el,1}] u_{2,0,0})$$

vanishes by the selection rules (32) and (30).

Suppose now that $n \geq 3$. We have to prove that there is an $i < j = n-1$ such that for all $\phi \in \operatorname{Ran} P_{el,j}$

$$\sum_{\upsilon=x,y,z} \|P_{el,i} p_\upsilon \phi\|^2 > 0.$$

Since $\operatorname{Im} Z$ is diagonal in the basis $\{u_{n,m,l} | l = 0 \ldots n-1,\ m = -l, \ldots, l\}$, it suffices to show

$$\sum_{\upsilon=x,y,z} \|P_{el,i} p_\upsilon u_{n,l,m}\|^2 > 0$$

for all $0 \leq l \leq n-1$ and $-l \leq m \leq l$. For the case $l = 0$, $m = 0$ it follows from equations (31) and (29) that the transition $(n,0,0) \to (2,1,0)$ is an allowed electric dipole transition, since $z^{n,0,0}_{2,1,0} > 0$. Consequently $(u_{n,0,0}, \operatorname{Im} Z u_{n,0,0}) > 0$.

Thus, it suffices to consider the case $l > 0$. The proof is by contradiction. Assume that $\sum_{\upsilon=x,y,z} \|P_{el,i} p_\upsilon u_{n,l,m}\|^2 = 0$ for all $i < j = n-1$ and some l, m. This would imply that for $\upsilon = x, y, z$

$$(p_\upsilon u_{n,l,m}, H_{el} p_\upsilon u_{n,l,m}) \geq E_j (p_\upsilon u_{n,l,m}, p_\upsilon u_{n,l,m}).$$

For $l > 0$, it is easy to see by Equation (26) that $p_\upsilon u_{n,l,m} \in \operatorname{Dom}(H_{el})$ and, using partial integration and the fact that $u_{n,l,m}(0) = 0$, we see that

$$\sum_{\upsilon=x,y,z} (p_\upsilon u_{n,l,m}, H_{el} p_\upsilon u_{n,l,m}) = E_j \sum_{\upsilon=x,y,z} (p_\upsilon u_{n,l,m}, p_\upsilon u_{n,l,m}).$$

Thus, we conclude by the variational principle that

$$H_{el} p_\upsilon u_{n,l,m} = E_j p_\upsilon u_{n,l,m}.$$

However,

$$E_j p_\upsilon u_{n,l,m} = H_{el} p_\upsilon u_{n,l,m} = E_j p_\upsilon u_{n,l,m} + [H_{el}, p_\upsilon] u_{n,l,m}$$

for $\upsilon = x, y, z$ and

$$[H_{el}, p_x] = -i \frac{x}{r^3}$$

with $r = \sqrt{x^2 + y^2 + z^2}$, so that we arrive at a contradiction.

$\square$

B.4. **Numerical Illustration.** In this subsection we give explicit numerical values for the matrix $\operatorname{Im} Z$ for the case $n = 3$ setting the cutoff function κ identically equal to one. Using Maple and the explicit form of the eigenfunctions in equation (27), we calculate the matrices $P_{el,0} x P_{el,2}$ and $P_{el,1} x P_{el,2}$ as well as the corresponding matrices for the coordinates y and z, where $P_{el,0}$ is the projection onto the groundstate, $P_{el,1}$ the projection onto the eigenspace belonging to $\mathfrak{E}_2$, and $P_{el,2}$ the projection onto the eigenspace belonging to $\mathfrak{E}_3$. With these matrices, we calculate $\operatorname{Im} Z$ according to equation (12). The numerical values for other principal quantum numbers could be calculated in the same way.

The matrix $\operatorname{Im} Z$ (and also Z) is diagonal in the basis $\{u_{3,l,m} | 0 \leq l \leq 2,\ -l \leq m \leq l\}$. The diagonal elements depend only on l, but not on m. We find $(u_{3,0,0}, \operatorname{Im} Z u_{3,0,0}) = \frac{192}{1953125}$, $(u_{3,1,m}, \operatorname{Im} Z u_{3,1,m}) = \frac{738423}{250000000}$ for $-1 \leq m \leq 1$,

and $(u_{3,2,m}, \mathrm{Im}\, Z u_{3,2,m}) = \frac{49152}{48828125}$ for $-2 \leq m \leq 2$. Let us remark that the eigenvalues of $2 \cdot (2\alpha^5 m\mathfrak{c}^2/\hbar)\mathrm{Im}\, Z$ are precisely the inverse lifetimes $\tau_{n,l,m}^{-1}$ of the corresponding eigenstates of the hydrogen atom. The additional factor two is due to the fact that lifetimes are defined via survival probabilities and not via survival amplitudes. Inserting $\alpha = 7.29735\cdot 10^{-3}$, $m = 9.10939\cdot 10^{-31} kg$, $\mathfrak{c} = 2.99792\cdot 10^8 m/s$ and $\hbar = 1.05457 \cdot 10^{-34} Js$ we find $\tau_{3,0,0} = 1.58303 \cdot 10^{-7} s$, $\tau_{3,1,m} = 5.26860 \cdot 10^{-9} s$ for $-1 \leq m \leq 1$, and $\tau_{3,2,m} = 1.54593\cdot 10^{-8} s$ for $-2 \leq m \leq 2$. Experimental values for these lifetimes are not very precise. We quote a value of $\tau_{3,1,m} = (5.5 \pm 0.2) \times 10^{-9} s$ given in [8]. [7] find a value of $\tau_{3,1,m} = (5.58 \pm 0.13) \times 10^{-9} s$ and [12] find $\tau_{3,1,m} = (5.41 \pm 0.18) \times 10^{-9} s$. Notice that the experimental values are in reasonable agreement with the calculated value.

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References

[1] V. Bach, J. Fröhlich, and I. M. Sigal. Mathematical theory of nonrelativistic matter and radiation. *Lett. Math. Phys.*, 34(3):183–201, 1995.
[2] V. Bach, J. Fröhlich, and I.M. Sigal. Spectral analysis for systems of atoms and molecules coupled to the quantized radiation field. Preprint, mp_arc 98-728, 1998.
[3] Volker Bach, Jürg Fröhlich, and Israel Michael Sigal. Quantum electrodynamics of confined nonrelativistic particles. *Adv. Math.*, 137(2):299–395, 1998.
[4] Volker Bach, Jürg Fröhlich, and Israel Michael Sigal. Spectral analysis for systems of atoms and molecules coupled to the quantized radiation field. *Comm. Math. Phys.*, 207(2):249–290, 1999.
[5] Volker Bach, Jürg Fröhlich, Israel Michael Sigal, and Avy Soffer. Positive commutators and the spectrum of Pauli-Fierz Hamiltonian of atoms and molecules. *Comm. Math. Phys.*, 207(3):557–587, 1999.
[6] Hans A. Bethe and Edwin E. Salpeter. *Quantum mechanics of one- and two-electron atoms.* Berlin-Göttingen-Heidelberg: Springer-Verlag. VIII, 368 pp. , 1957.
[7] William S. Bickel and Allan S. Goodman. Mean lives of the 2p and 3p levels in atomic hydrogen. *Physical Review*, 148(2):1–4, August 1970.
[8] E. L. Chupp, L. W. Dotchin, and D. J. Pegg. Radiative mean-life measurements of some atomic-hydrogen excited states using beam-foil excitation. *Physical Review*, 175(1), November 1968.
[9] Claude Cohen-Tannoudji, Jacques Dupont-Roc, and Gilbert Grynberg. *Atom-Photon Interactions – Basic Processes and Applications.* John Wiley and Sons, Inc., 1992.
[10] Claude Cohen-Tannoudji, Jacques Dupont-Roc, and Gilbert Grynberg. *Photons & Atoms.* WILEY-VCH Verlag GmbH& Co. KGaA, 2004.
[11] E. B. Davies. The functional calculus. *J. London Math. Soc. (2)*, 52(1):166–176, 1995.
[12] R. C. Etherton, L. M. Beyer, W. E. Maddox, and L. B. Bridwell. Lifetimes of 3p, 4p, and 5p states in atomic hydrogen. *Physical Review A*, 2(6):2177–2179, December 1970.
[13] W. Gordon. Zur Berechnung der Matrizen beim Wasserstoffatom. *Annalen d. Physik*, 5(2):1031–1056, 1929.

[14] B. Helffer and J. Sjöstrand. Équation de Schrödinger avec champ magnétique et équation de Harper. In *Schrödinger operators (Sønderborg, 1988)*, volume 345 of *Lecture Notes in Phys.*, pages 118–197. Springer, Berlin, 1989.

[15] Walter Hunziker. Resonances, metastable states and exponential decay laws in perturbation theory. *Comm. Math. Phys.*, 132(1):177–188, 1990.

[16] V. Jakšić and C.-A. Pillet. On a model for quantum friction. I. Fermi's golden rule and dynamics at zero temperature. *Ann. Inst. H. Poincaré Phys. Théor.*, 62(1):47–68, 1995.

[17] Christopher King. Resonant decay of a two state atom interacting with a massless non-relativistic quantised scalar field. *Comm. Math. Phys.*, 165(3):569–594, 1994.

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